Uncovering non-Fermi-liquid behaviour in Hund metals




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arXiv:1808.09936v3 [accepted in Ann. Phys., 2019]

arXiv:1708.05752v3 [accepted in Nature Comm., 2019]


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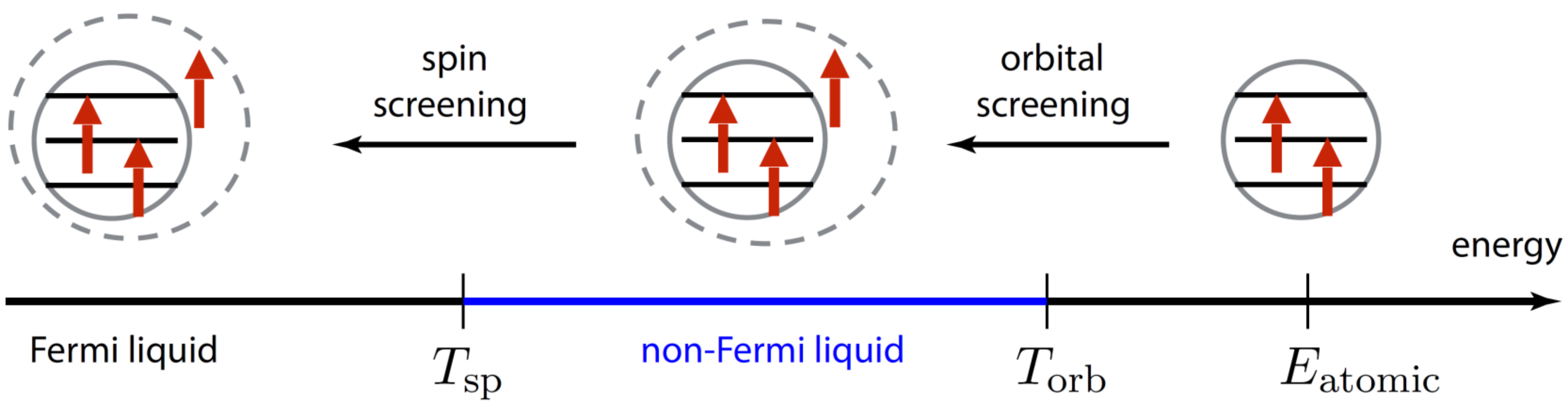

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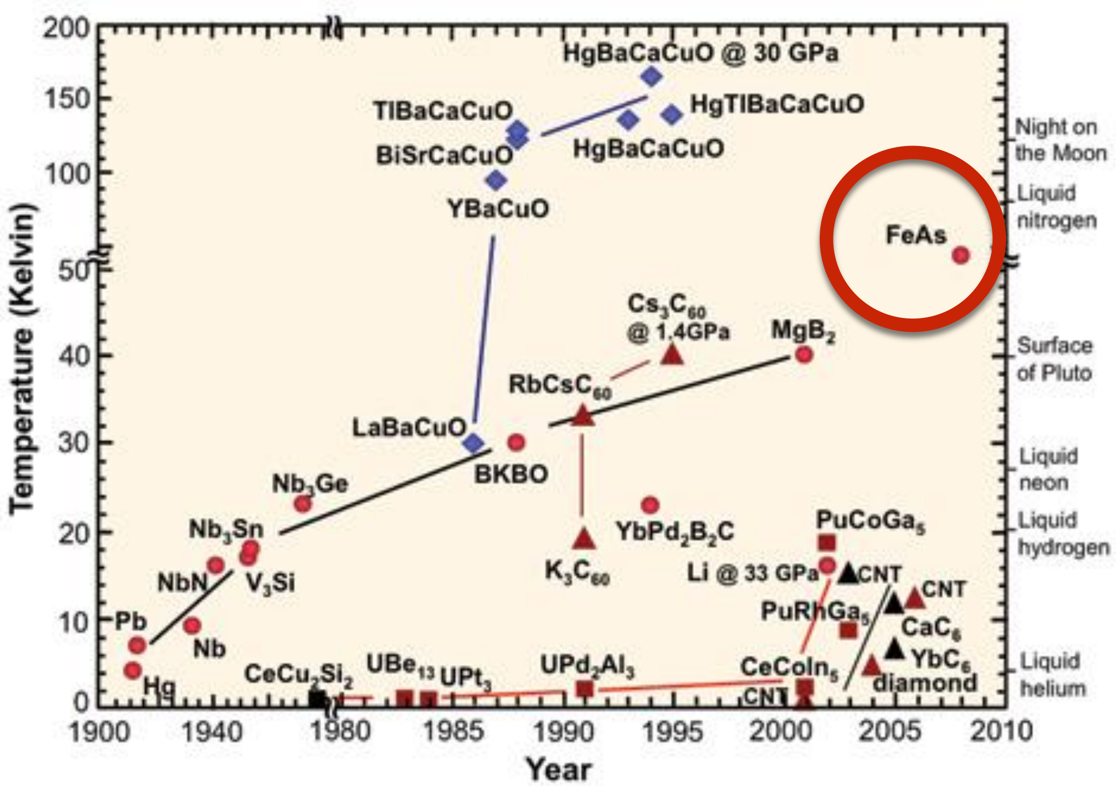
Motivation: iron pnictides

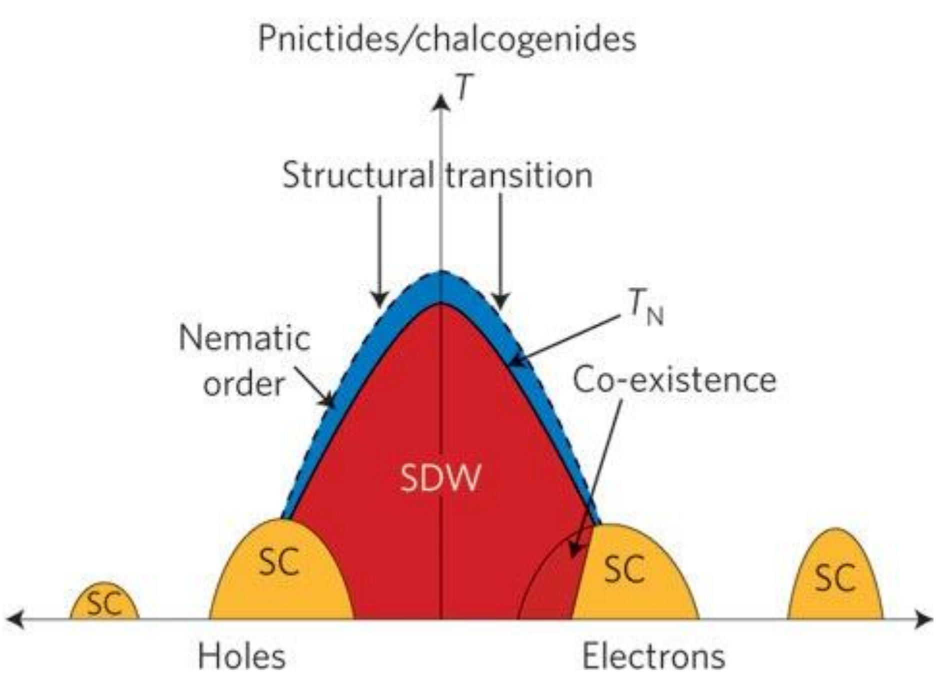


http://www.globalspec.com

Discovery of iron-based high-T_c superconductors in 2008:
La[$O_{1-x}F_x$]FeAs (x = 0.05−0.12) with T_c = 26 K

Hideo Hosono

J. Am. Chem. Soc. 130 (11), 3296-3297 (2008)



Nature Physics 7, 272–276 (2011)

anomalous properties also in the normal state

↓

pairing mechanism ???

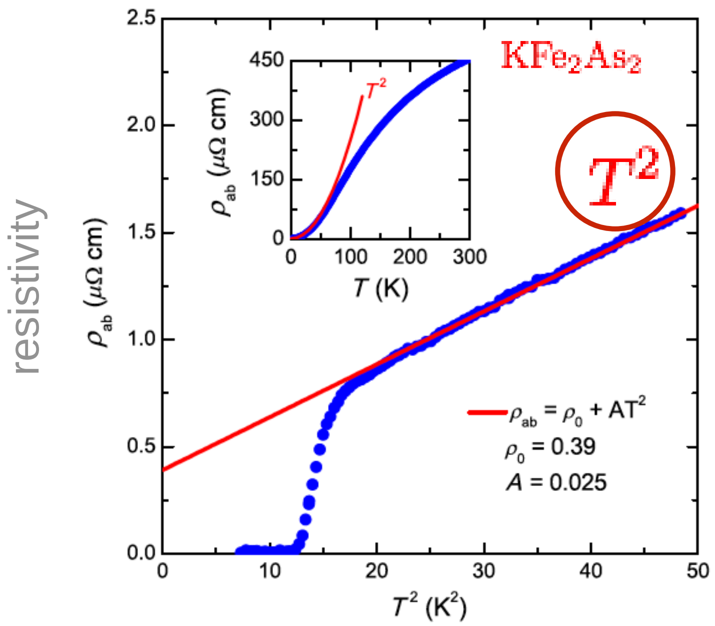
↑

multi-band materials:
role of orbitals/bands?
role of spins and their fluctuations?

Iron pnictides have anomalous normal-state properties

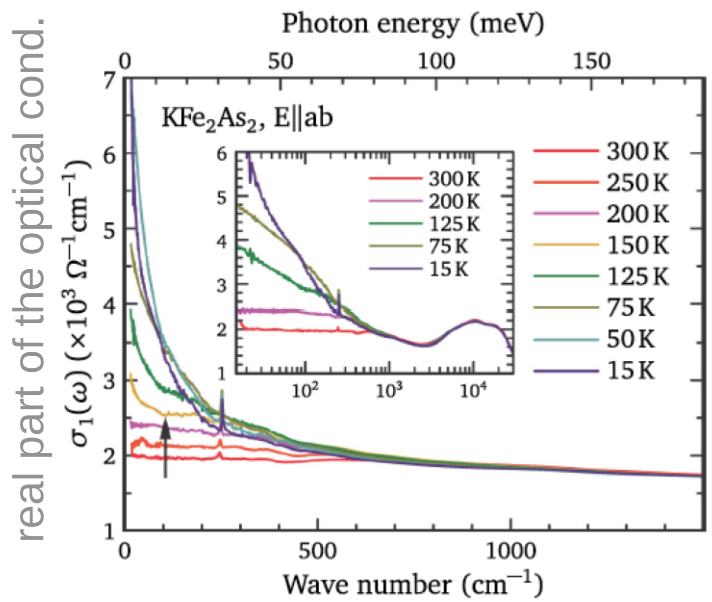
experiments: significant mass enhancement + coherence-incoherence crossover → strong correlations!?!

Hardy *et al.*, PRL **111**, 027002 (2013)



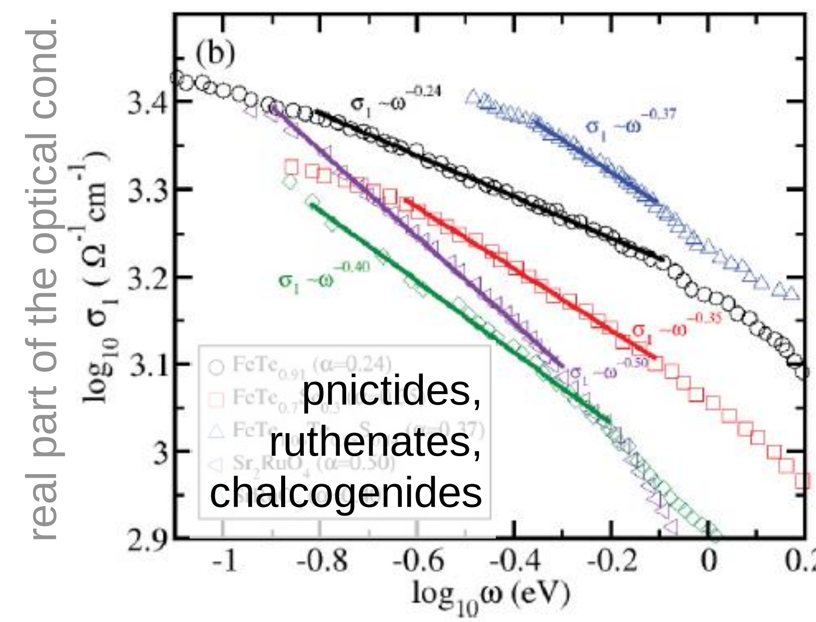
temperature

Yang *et al.*, PRB **96**, 201108 (2017)



real frequency

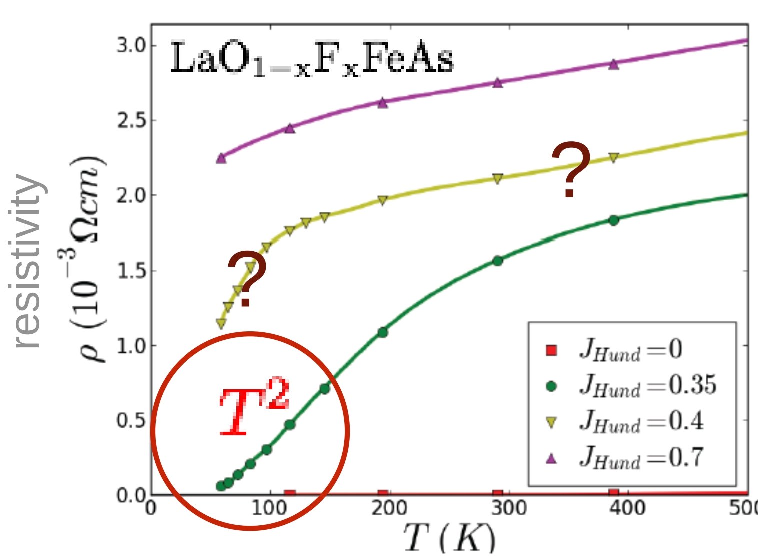
Lee *et al.*, PRB 67, 113101 (2003)



real frequency

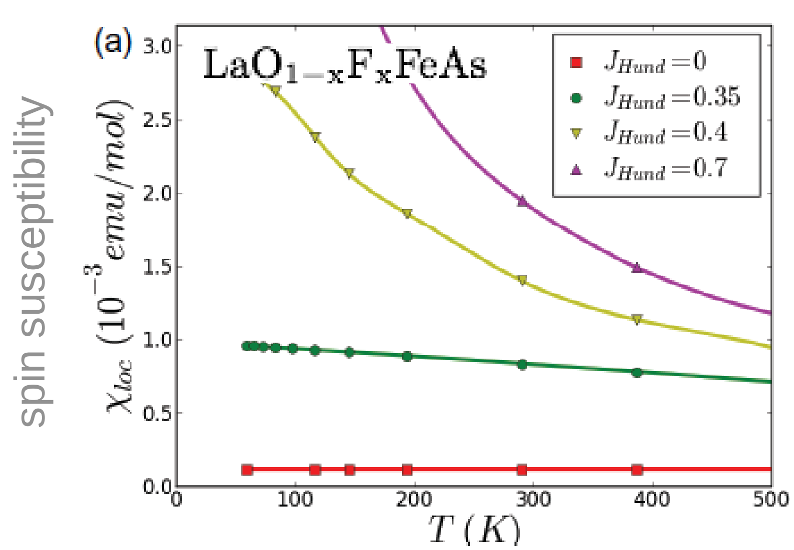
DFT+DMFT+QMC: ?!? major ingredient: Hund's coupling J !

Haule & Kotliar, NJP **11**, 025021 (2009)



temperature

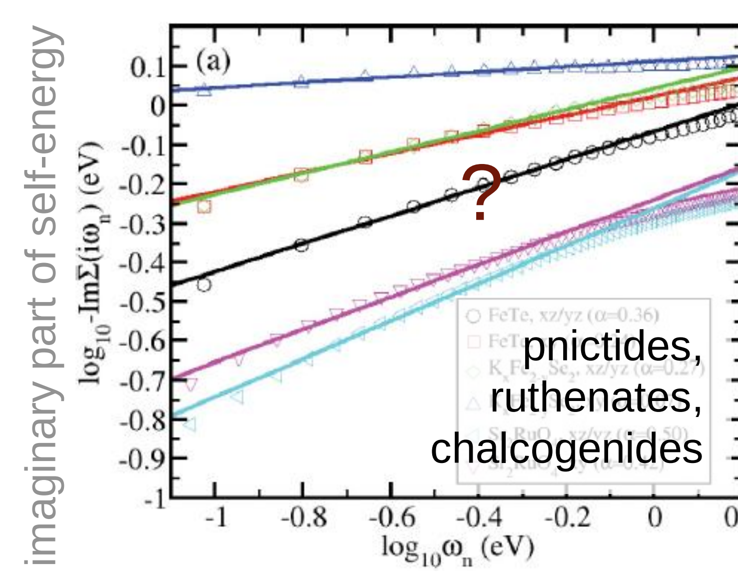
resistivity increases with J



temperature

susceptibility increases with J

Yin *et al.*, PRB **86**, 195141 (2012)



Matsubara frequency

Summary: iron pnictides in normal state are bad metals

- iron pnictides in normal state are bad metals:
  - low coherence scales T_{FL}
  - large effective masses
  - small quasiparticle weight

- multi-orbital, wide-band materials:
  Coulomb U smaller than for single-orbital, narrow-band materials

- new ingredient: Hund's coupling J:
  favors alignment of spins in different orbitals

- one charge away from half-filling (Fe 3d6 for 5 d-orbitals)

- non-trivial interplay of spin and orbital degrees of freedom

- what is the role of U vs. J ?
  "Mottness vs. Hundness"

- similar issues arise for other multi-band bad-metal materials:
  chalcogenide superconductors,
  ruthenates…

Minimal model for Hund metals: 3-band Hubbard-Hund model

3-band Hubbard model with Hund's coupling:

$$\hat{H}_{\mathrm{HHM}} = \sum_i \left(-\mu \hat{N}_i + \hat{H}_{\mathrm{int}}[\hat{d}^\dagger_{im\sigma}]\right) + \sum_{\langle ij \rangle m\sigma} t\, \hat{d}^\dagger_{im\sigma} \hat{d}_{jm\sigma}$$

$$\hat{N}_i = \sum_{m\sigma} \hat{d}^\dagger_{im\sigma} \hat{d}_{im\sigma}$$

$$\hat{H}_{\mathrm{int}}[\hat{d}^\dagger_{im\sigma}] = \tfrac{3}{4} J_H \hat{N}_i + \tfrac{1}{2}(U - \tfrac{1}{2} J_H)\hat{N}_i(\hat{N}_i - 1) - J_H \hat{\mathbf{S}}_i^2$$

$$\hat{S}_i^\alpha = \tfrac{1}{2} \sum_{m\sigma\sigma'} \hat{d}^\dagger_{im\sigma} \sigma^\alpha_{\sigma\sigma'} \hat{d}_{im\sigma} \qquad \mathrm{Tr}[\sigma^\alpha \sigma^\beta] = 2\delta_{\alpha\beta}$$

Werner, Gull, Troyer, Millis, PRL 2008
de' Medici, Mravlje, Georges, PRL 2011
Yin, Haule, Kotliar, PRB 2012
…

energy unit: t = 1

the 3 orbitals are degenerate

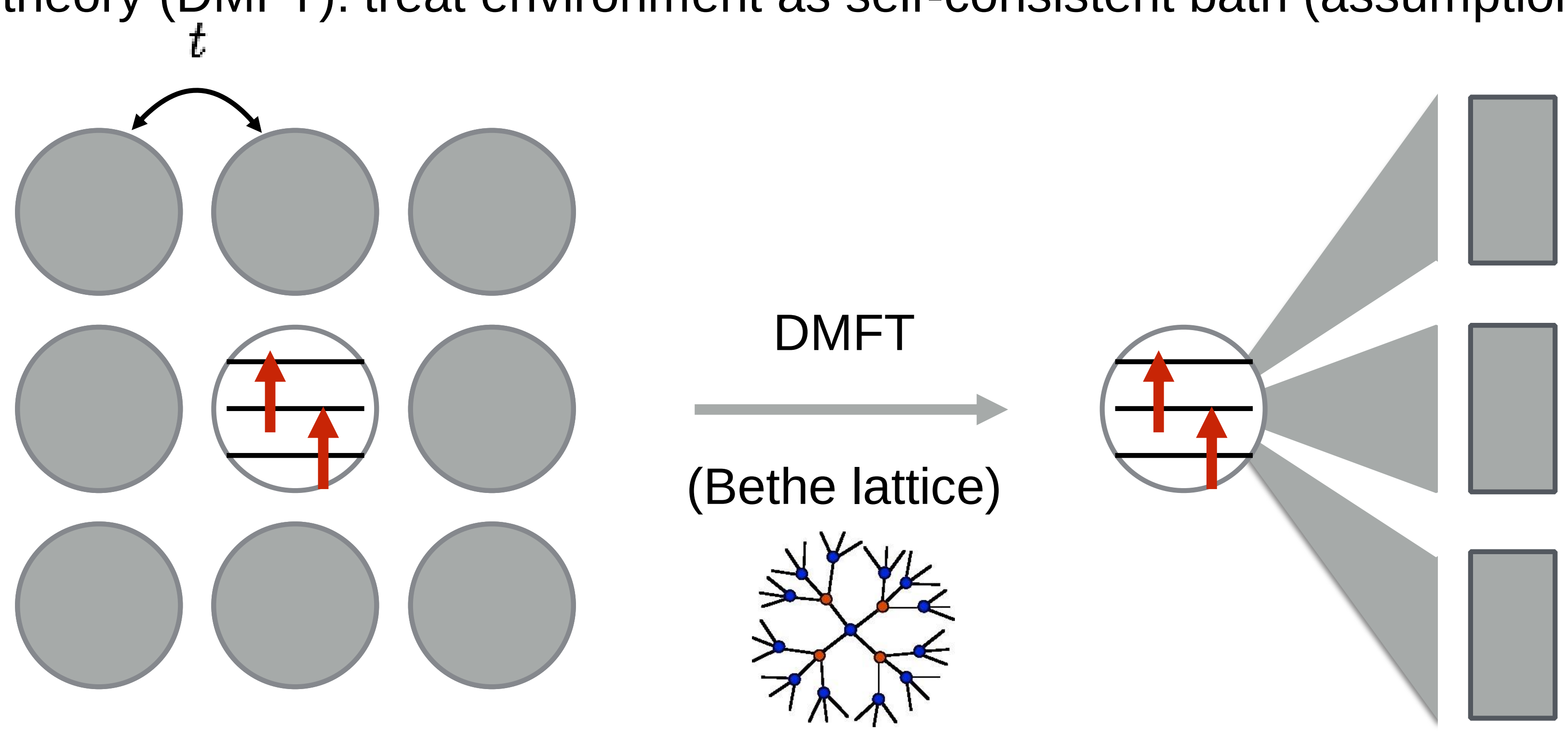
symmetry: $U(1)_{ch} \times SU(2)_{sp} \times SU(3)_{orb}$

Dynamical mean-field theory (DMFT): treat environment as self-consistent bath (assumption: local self-energy)

$n_d = \langle \hat{N}_i \rangle \simeq 2$

$m = 1, 2, 3$

$\sigma \in \{\uparrow, \downarrow\}$



self-consistent 3-band Anderson-Hund model (3AHM)

Quantum impurity solvers

Needed: real-frequency "quantum impurity solvers" that can treat 3-band models at very low temperatures!

Impurity solvers:

- exact diagonalization
- iterative perturbation theory
- diagrammatic schemes
- interpolation schemes
- continuous-time Quantum Monte Carlo (ctQMC)
- Numerical Renormalization Group (NRG)
- Density Matrix Renormalization Group (DMRG)
- Chebychev expansions with MPS (CheMPS)

  …

Currently most popular: ctQMC
 + very successful in general
 - increasingly costly with decreasing temperatures
 - analytical continuation for real-frequency data
 - sign problem for some models

Numerical Renormalization Group (NRG)
+ high spectral resolution at arbitrarily low energies
+ real-frequency data
+ arbitrary temperatures
+ no sign problem
- costs increase exponentially with number of bands

tremendous technical progress in recent years
+ complete many-body basis [1]
+ formulation in MPS language [2]
+ fdmNRG for highly accurate correlation functions at arbitrary temperatures [3]
+ improved treatment of hybridization function [4]
+ …

for multi-band models
+ exploiting abelian and non-abelian symmetries:

$$\mathrm{U(1)_{ch}} \times \mathrm{SU(2)_{sp}} \times \mathrm{SU(3)_{orb}}$$ [5]

+ interleaved NRG for non-symmetric models
+ adaptive broadening improves spectral resolution [8]

[1] Anders, Schiller, PRL 95 (2005), PRB 74 (2006)
[2] Weichselbaum, Verstraete, Schollwöck, Cirac, von Delft, cond-mat/0504305 (2005); Weichselbaum, PRB,86 (2012)
[3] Peters, Pruschke, Anders, PRB 74 (2006); Weichselbaum, von Delft, PRL 99 (2007)
[4] Zitko, Computer Phys. Comm. 180 (2009); Zitko, Pruschke, PRB 79 (2009)
[5] Toth, Moca, Legeza, Zarand, PRB 78 (2008); Weichselbaum, Ann. Phys. 327 (2012)
[6] Mitchell, Galpin, Wilson-Fletcher, Logan, Bulla, PRB 89 (2014)
[7] Stadler, Mitchell, von Delft, Weichselbaum, PRB, 93 (2016)
[8] Lee, Weichselbaum, PRB 94 (2016).

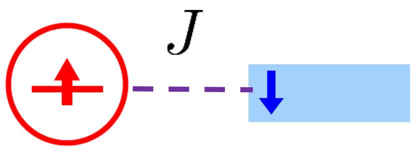
Andreas Weichselbaum

Outline

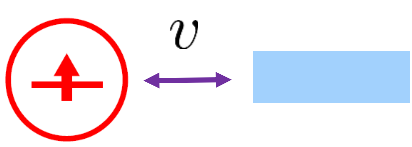
Introductory review: how does NRG work?

Impurity models

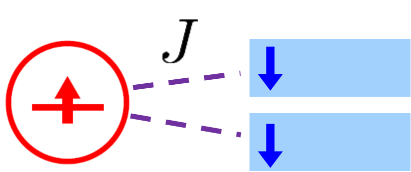
- Basics: spin screening in 1-channel Kondo (1CK) model



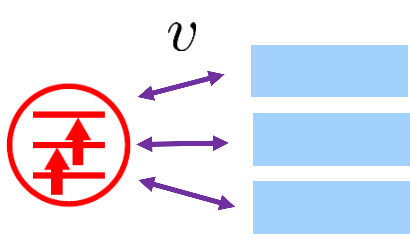
spin screening in 1-channel Anderson (1CA) model



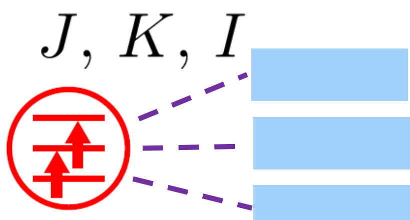
- NFL (spin): spin overscreening in 2-channel Kondo (2CK) model



- NFL (orbital) : orbital overscreening in 3-channel Anderson-Hund (3AH) model



orbital overscreening in 3-channel Kondo-Hund (3KH) model



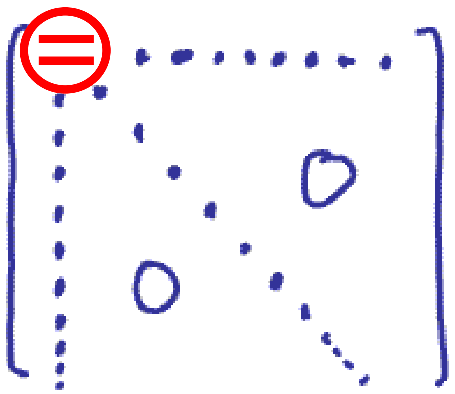
Back to DMRG…

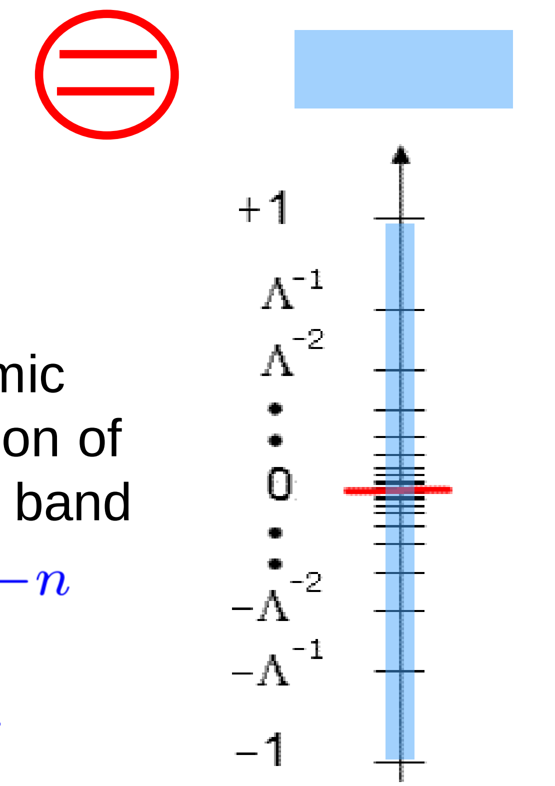
NRG: logarithmic discretization, Wilson chain

[Wilson, 1975]

$$H = H_0(d^\dagger, d) + \sum_k \varepsilon_k c_k^\dagger c_k + d^\dagger v \sum_k c_k + v \sum_k c_k^\dagger d$$

$$H_0 \equiv f_0 \qquad \qquad \qquad f_1$$





logarithmic discretization of conduction band

$$\xi_n \sim \Lambda^{-n}$$

$$\Lambda > 1$$

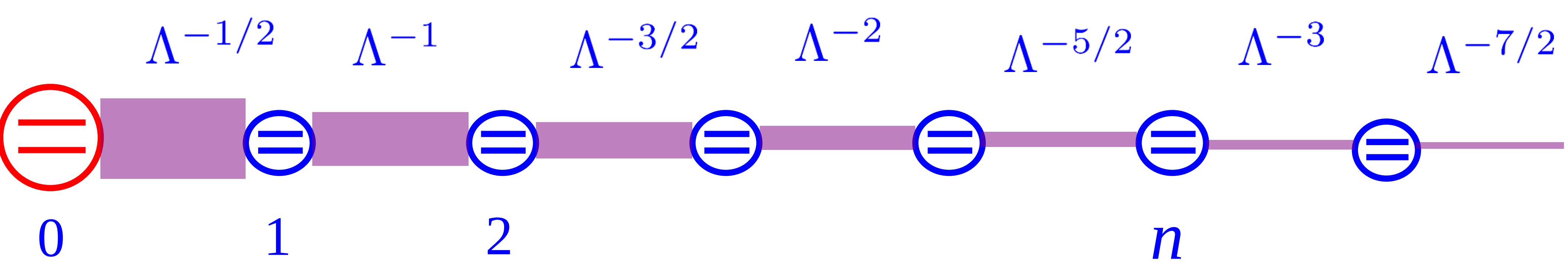
$$H = H_0(f_0^\dagger, f_0) + \sum_{n=1}^{\infty} t_n (f_n^\dagger f_{n-1} + f_{n-1}^\dagger f_n)$$

Wilson chain

$$t_n \sim \Lambda^{-n/2}$$

local state space:

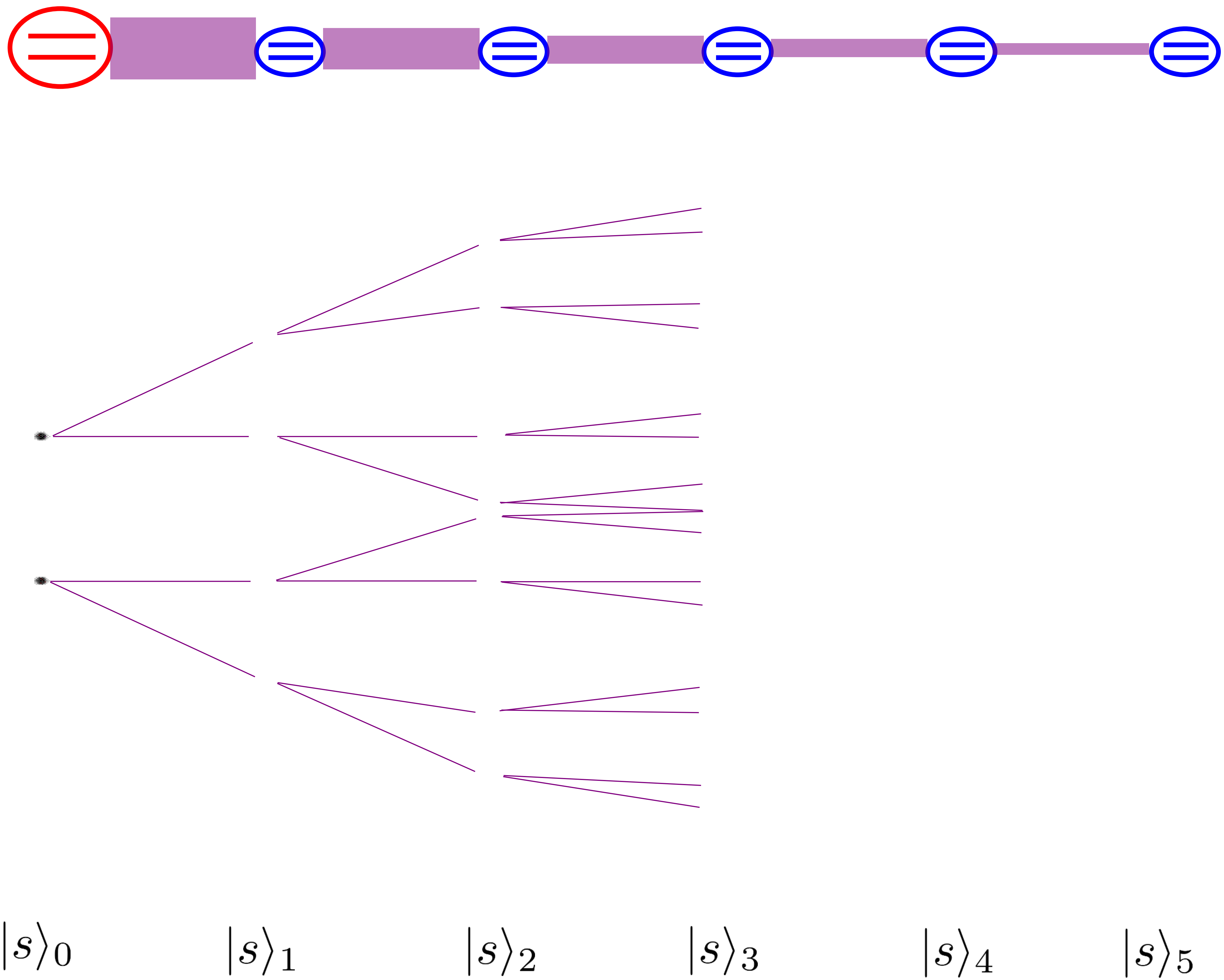
$$\sigma_n \in \{|0\rangle, |1\rangle\}$$



Diagonalize chain iteratively, discard high-energy states

NRG: iterative diagonalization

[Wilson, 1975]



complete basis
of exact
many-body
eigenstates of H

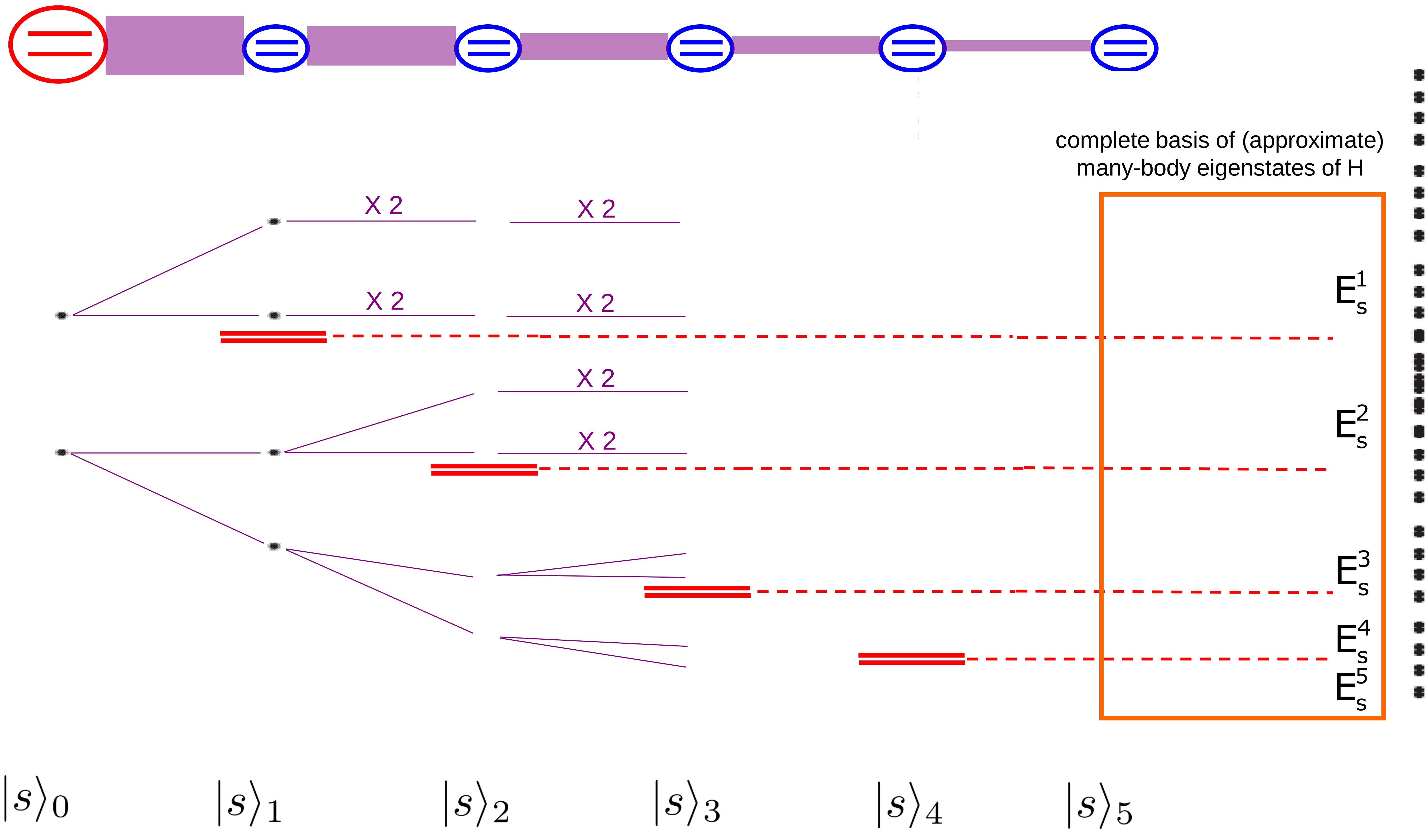
Dimension of
Hilbert space
grows as 2^n

Truncation
criterion
needed!

NRG: energy truncation, complete many-body basis

[Wilson, 1975]

truncate, and build complete many-body basis from discarded states, keeping track of degeneracies



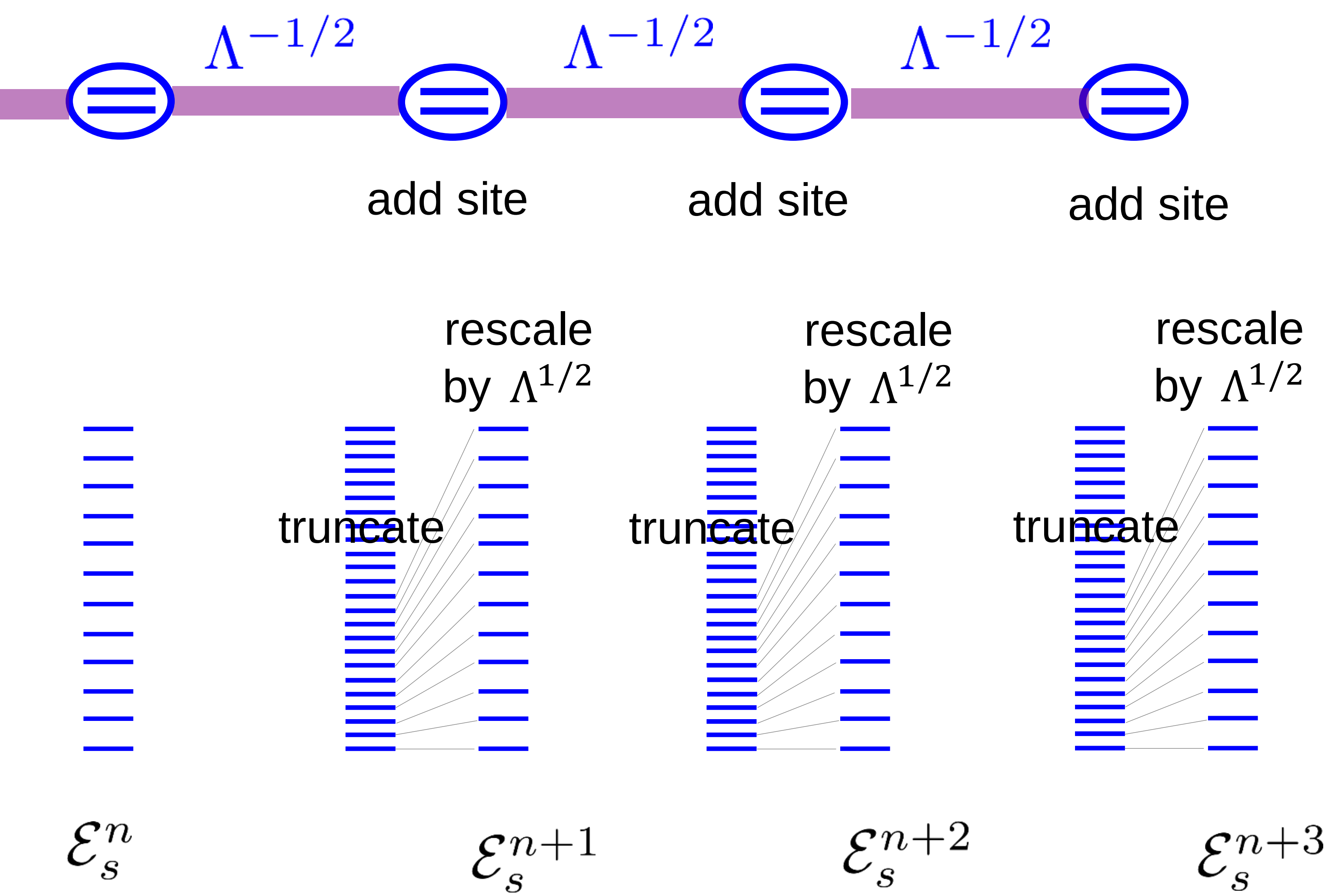
NRG: energy level flow diagram

[Wilson, 1975]

level splitting at iteration n : $\omega_n \simeq \Lambda^{-n/2} \sim \frac{1}{\text{effective system size}}$

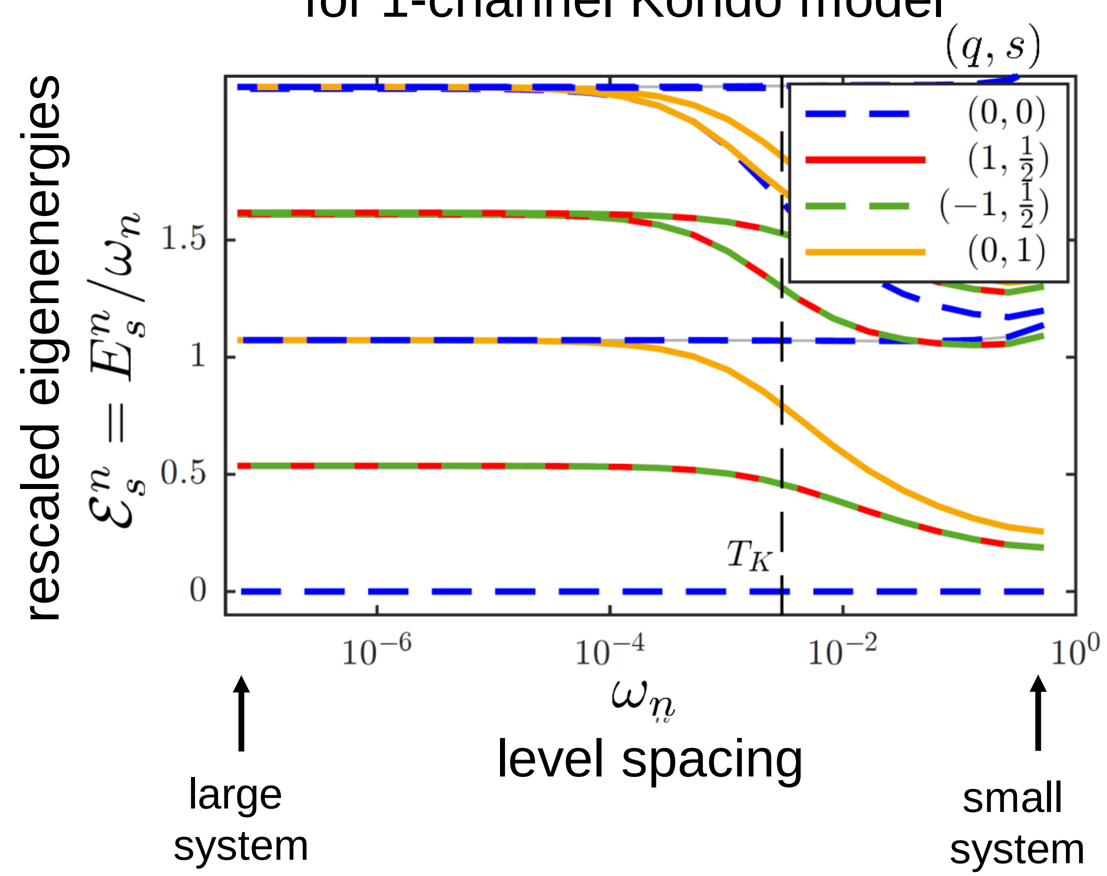
to maintain level splitting $\mathcal{O}(1)$, rescale eigenenergies: $\mathcal{E}_s^n \equiv E_s^n / \omega_n = \Lambda^{n/2} E_s^n$

in rescaled units, each new site perturbs previous spectrum by $\sim \Lambda^{-1/2}$



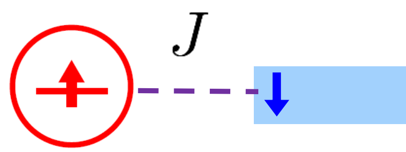
energy level flow diagram

for 1-channel Kondo model



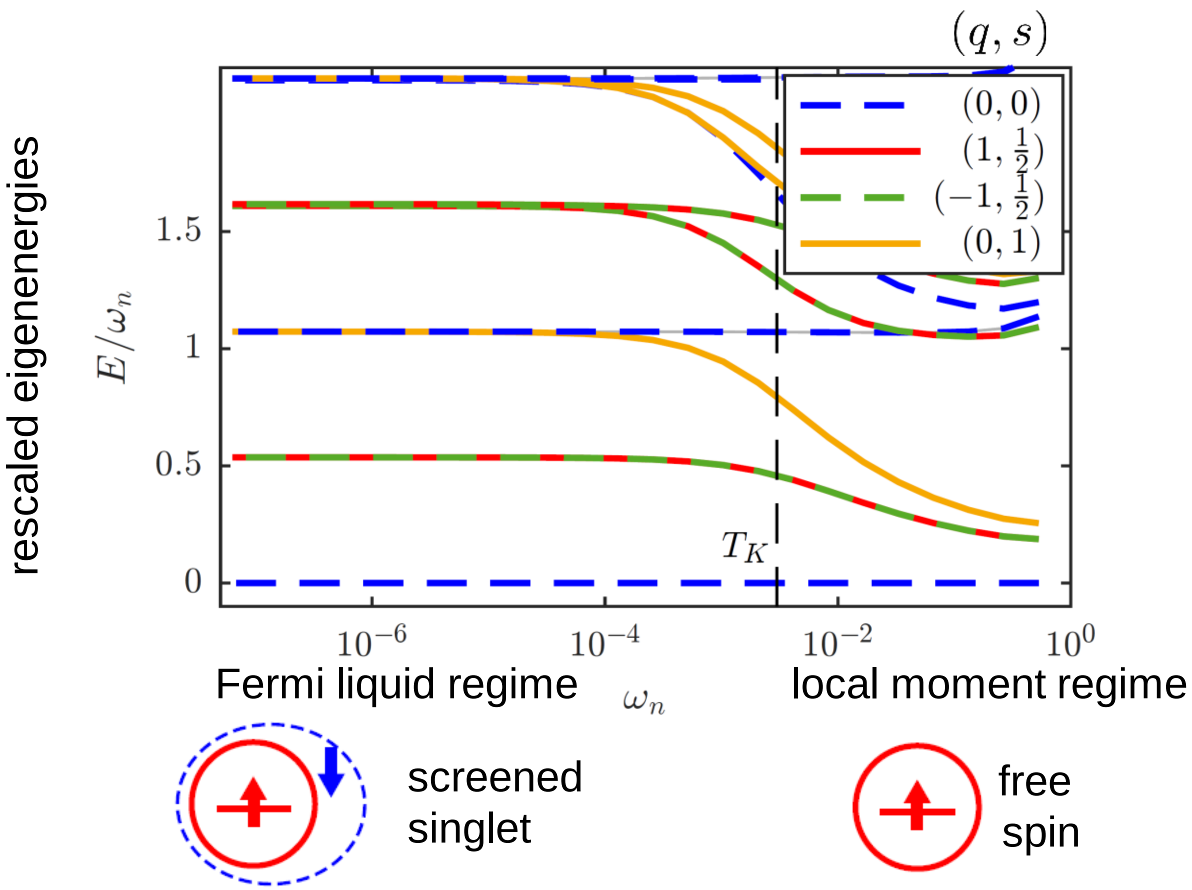
Basics: 1-channel Kondo model

$$H_{1\mathrm{CK}} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}$$

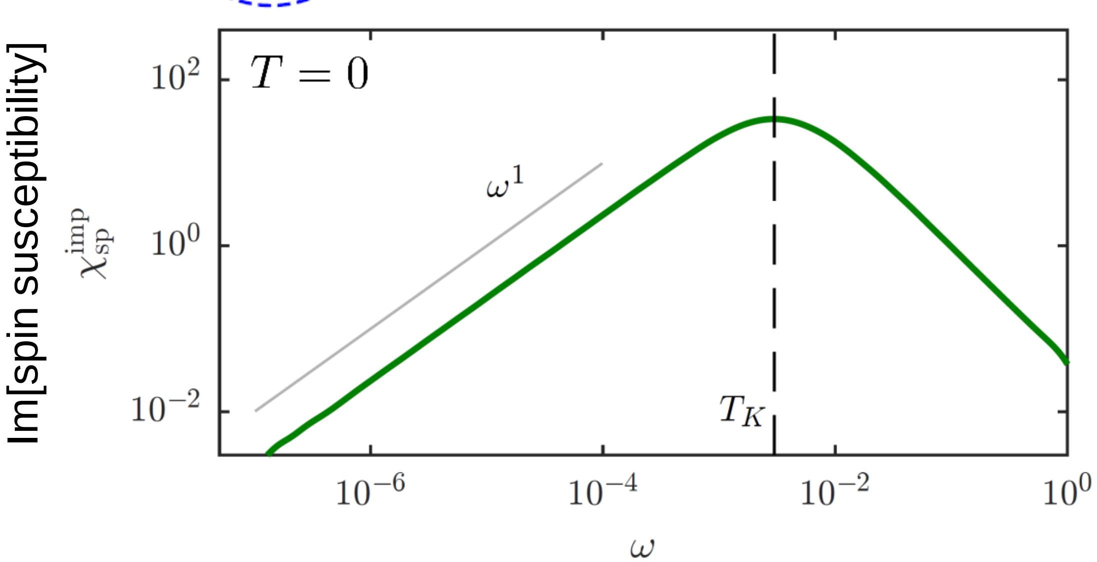


$$+ J\mathbf{S}\cdot\mathbf{J}_{\mathrm{sp}}$$

here $J^\alpha_{\mathrm{sp}} = \sum_{kk'} c^\dagger_{k\sigma}\sigma^\alpha_{\sigma\sigma'}c_{k'\sigma}$ is 'spin current' (conduction band spin at impurity site)



- spectrum changes qualitatively when level spacing ω_n drops below 'Kondo temperature, T_K
- high energies $(\omega_n \gg T_{\mathrm{K}})$: local moment regime
- low energies $(\omega_n \ll T_{\mathrm{K}})$: Fermi liquid regime
- ground state: impurity spin is screened by bath spin, forming spin singlet, $\langle \mathbf{S}_{\mathrm{imp}} \cdot \mathbf{s}_{\mathrm{band}} \rangle = 0$



$$\chi^{\mathrm{imp}}_{\mathrm{sp}}(\omega) \propto \langle \mathbf{S} || \mathbf{S} \rangle_\omega$$

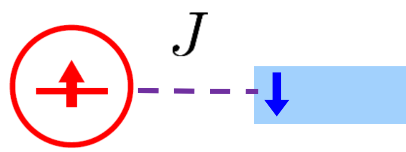
$$\propto \int \frac{dt}{2\pi}\, e^{i\omega t} \langle \mathbf{S}(t)\mathbf{S}(0)\rangle$$

$$= \sum_{s,s'} \left| \langle s'|\mathbf{S}|s\rangle \right|^2 \frac{e^{-\beta E_s}}{Z} \delta(\omega - E'_s + E_s))$$

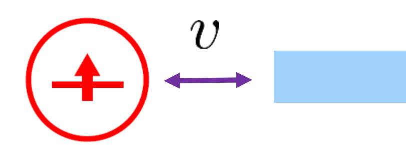
Lehmann representation, computable using complete basis

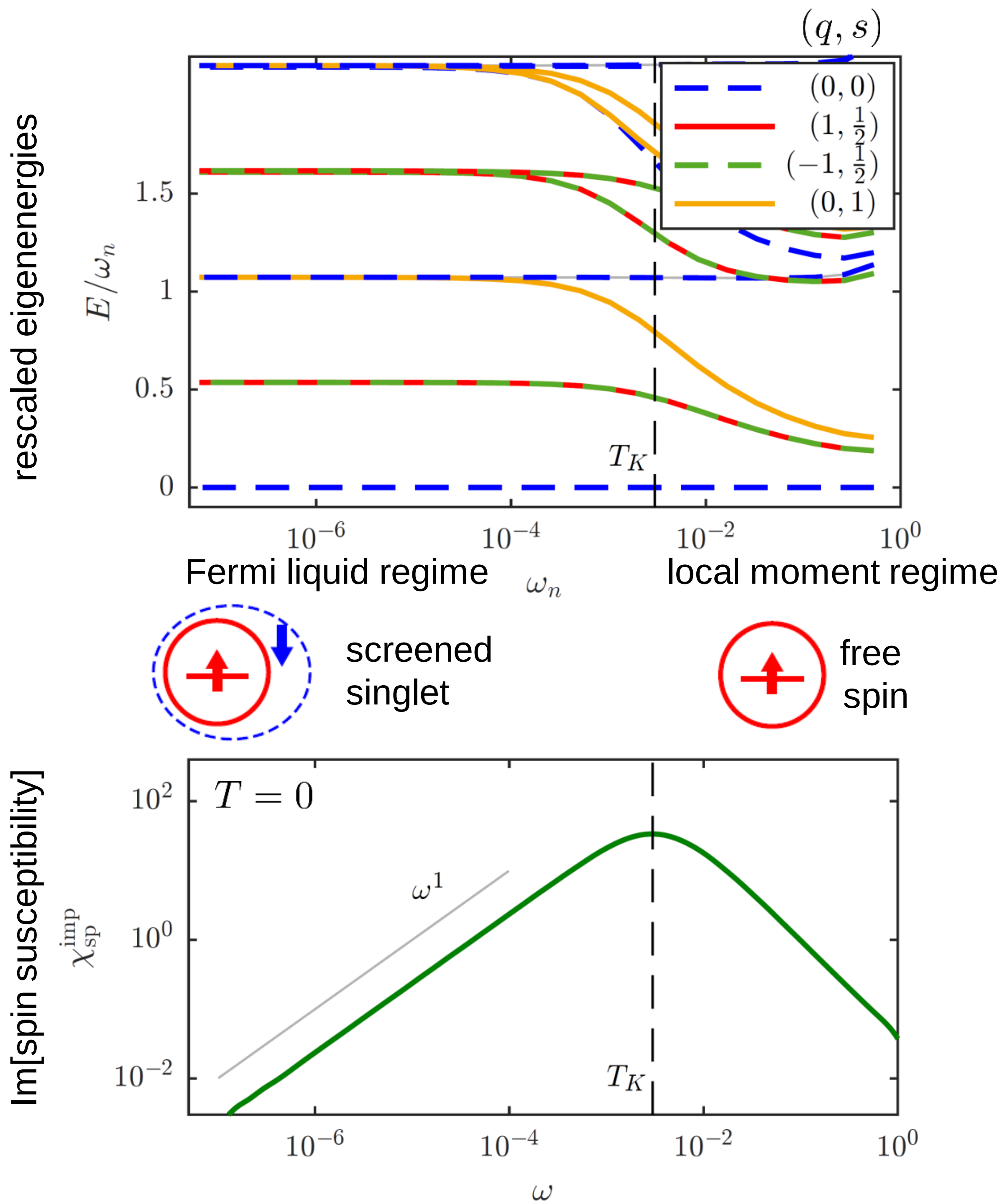
Basics: 1-channel Kondo vs. 1-channel Anderson model

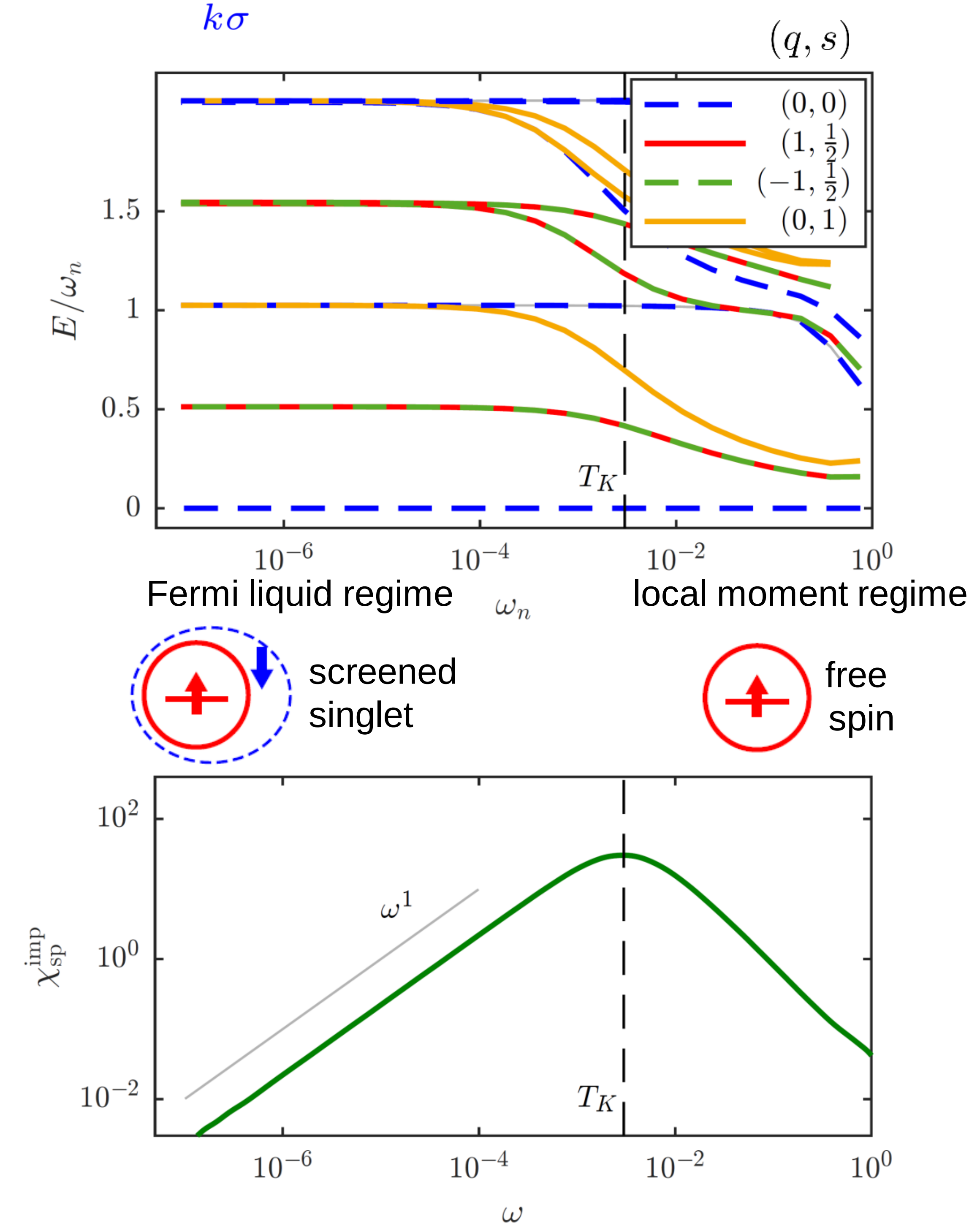
$$H_{1\mathrm{CK}} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J\,\mathbf{S}\cdot\mathbf{J}_{\mathrm{sp}}$$



$$H_{1\mathrm{CA}} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + v \sum_{k\sigma} \left(d^\dagger_\sigma c_{k\sigma} + c^\dagger_{k\sigma} d_\sigma\right) + U\,\hat{n}_\uparrow \hat{n}_\downarrow$$

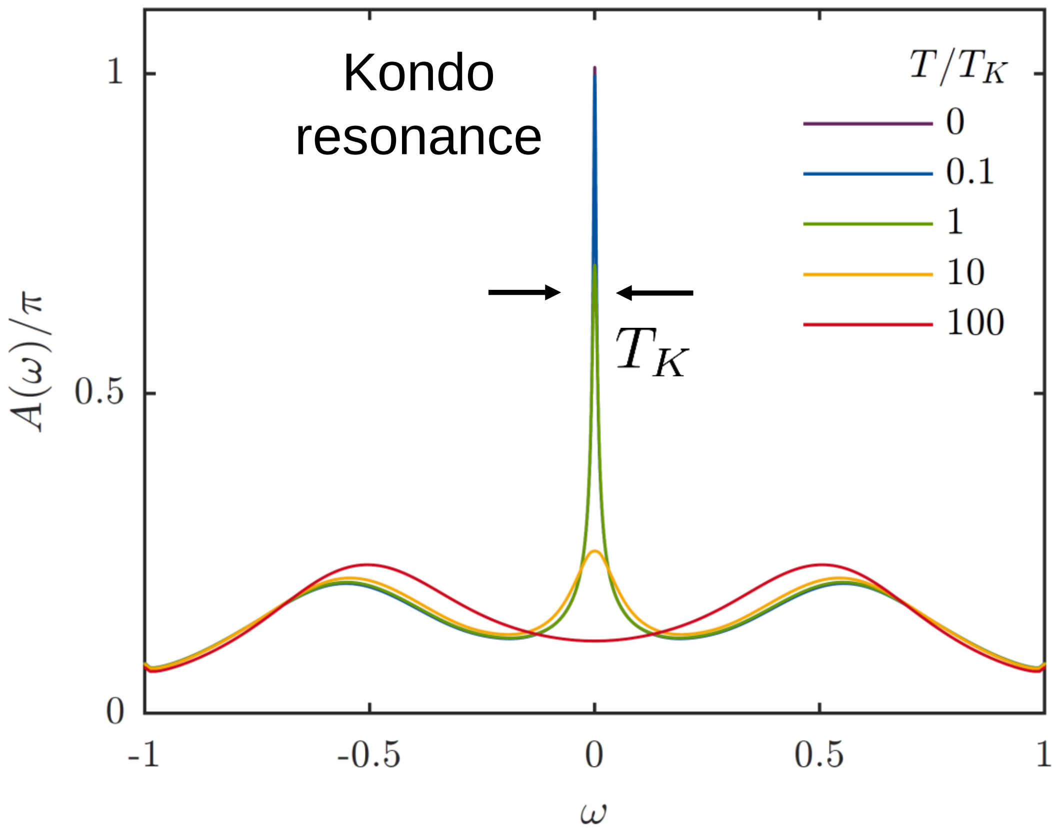


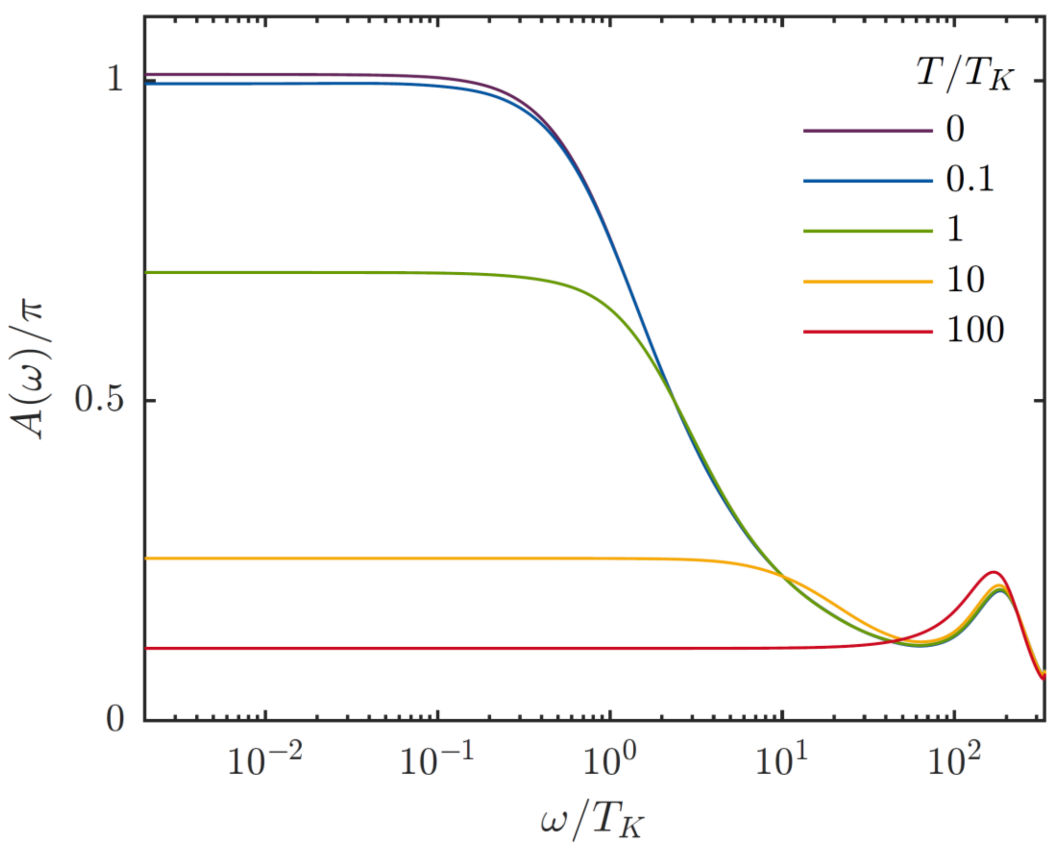




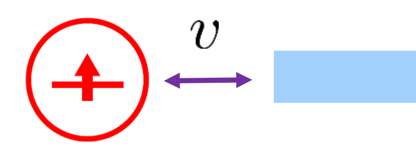
Basics: 1-channel Anderson model - local spectral function

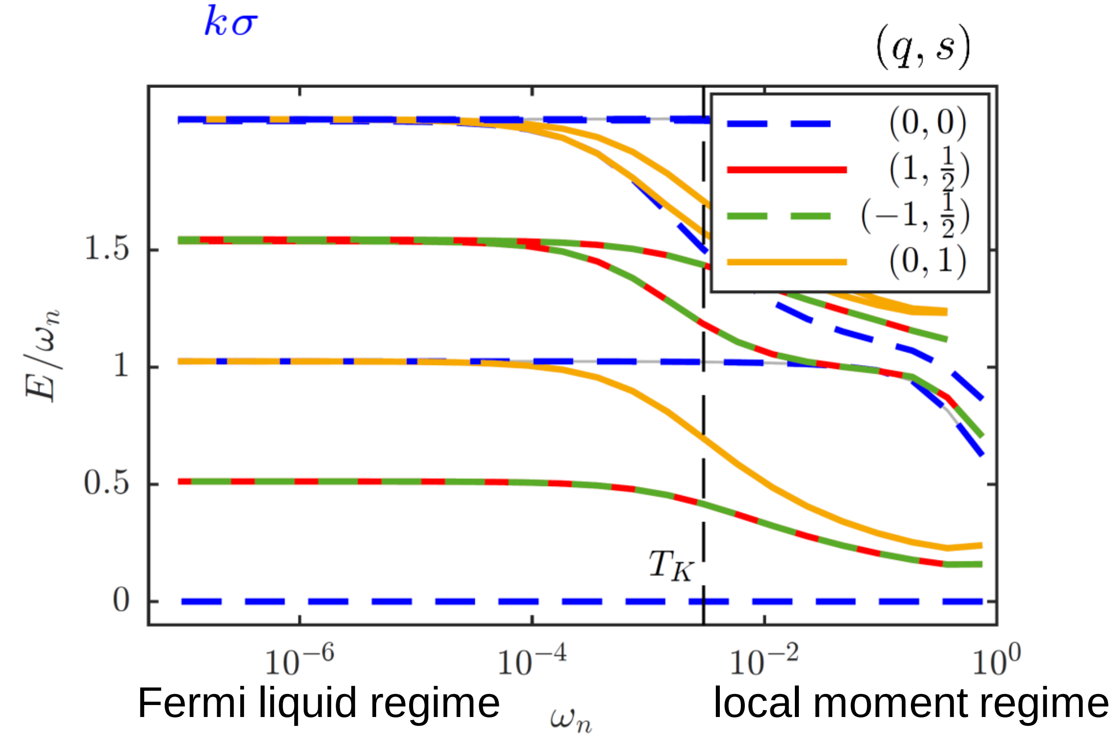
$$A(\omega) = -\mathrm{Im}\langle d_\sigma || d_\sigma^\dagger \rangle_\omega$$

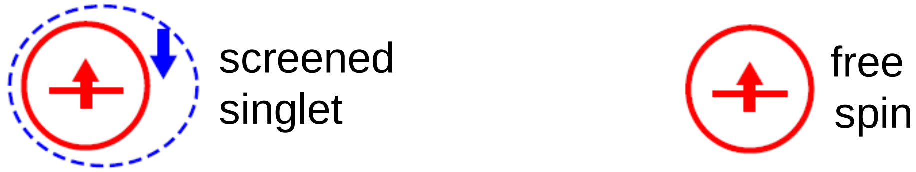


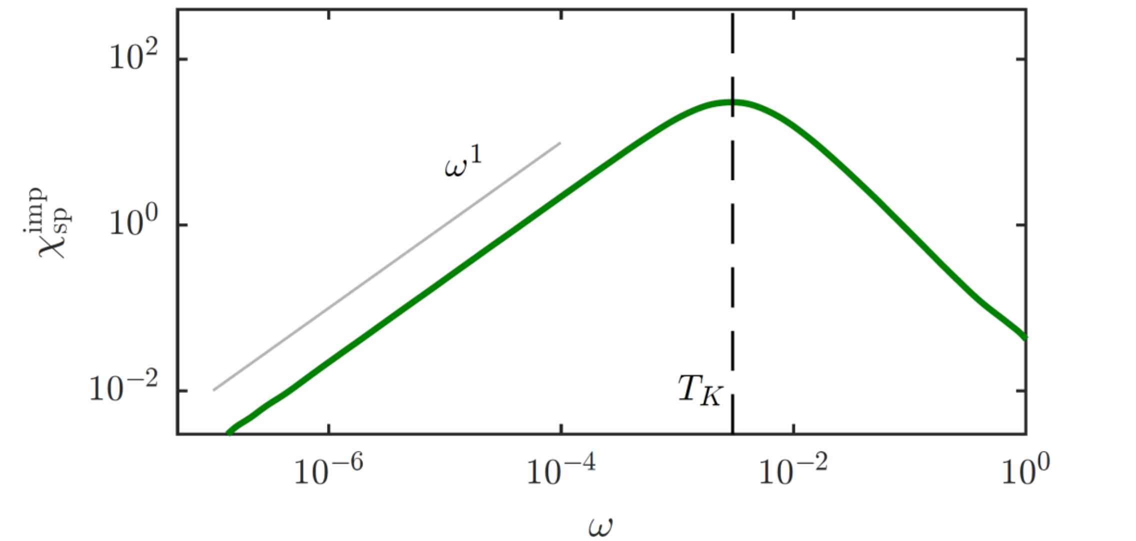


$$H_{1\mathrm{CA}} = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + v \sum_{k\sigma} (d_\sigma^\dagger c_{k\sigma} + c_{k\sigma}^\dagger d_\sigma) + U \hat{n}_\uparrow \hat{n}_\downarrow$$



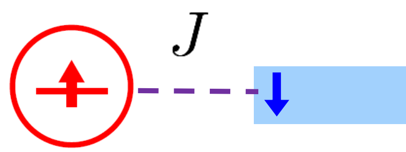




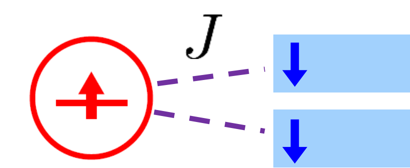


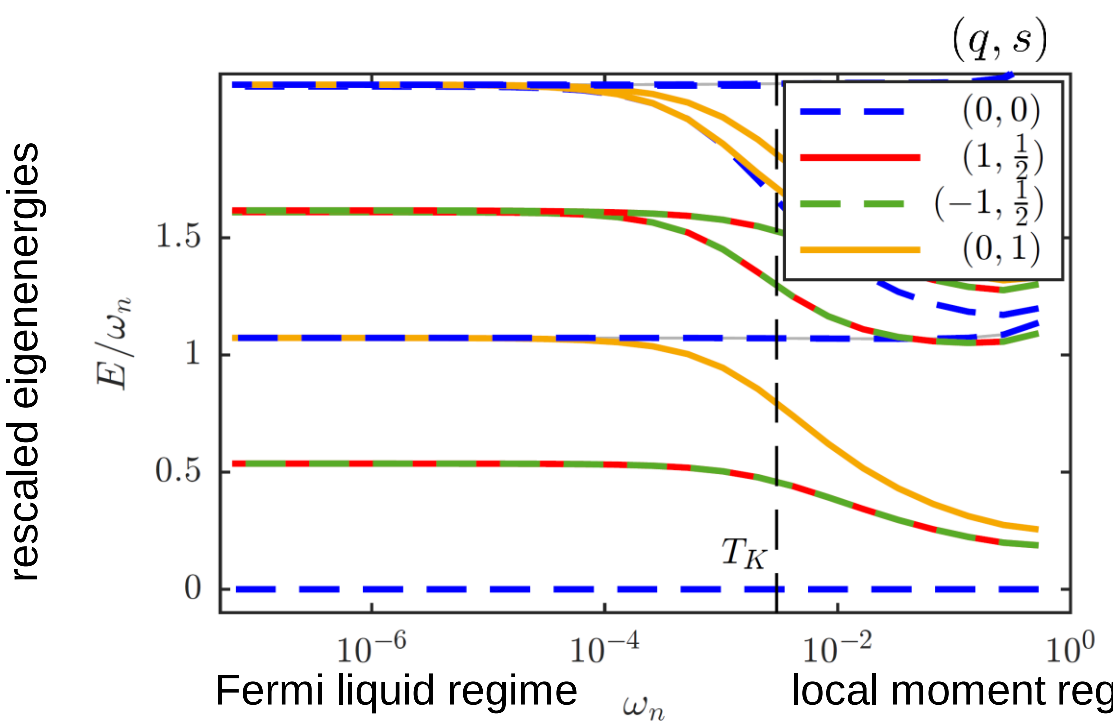
NFL (spin): 1-channel Kondo vs. 2-channel Kondo model

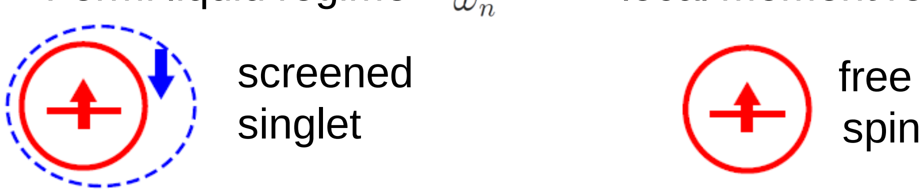
$$H_{1\mathrm{CK}} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J\mathbf{S}\cdot\mathbf{J}_{\mathrm{sp}}$$

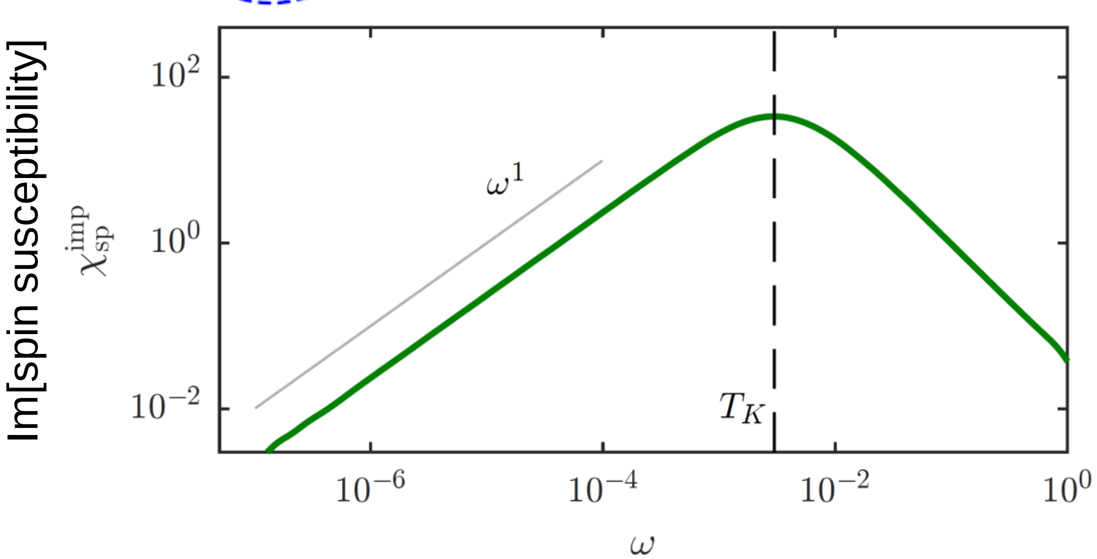


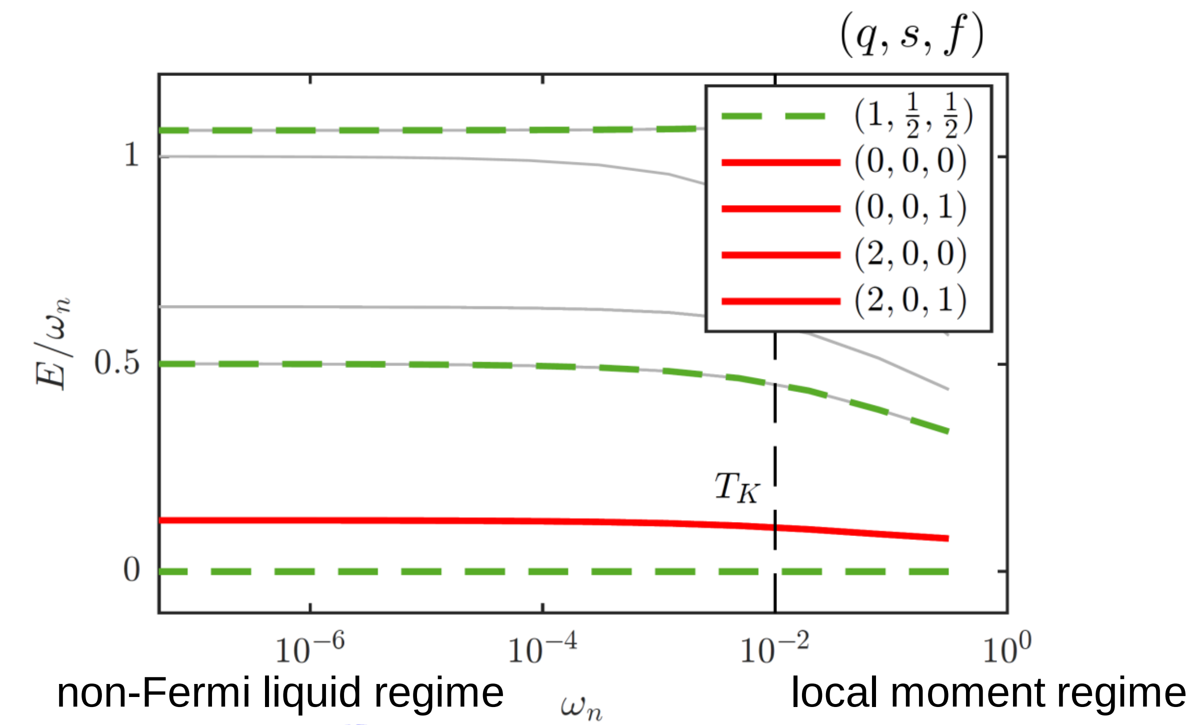
$$H_{2\mathrm{CK}} = \sum_{k\sigma} \sum_{m=1,2} \varepsilon_k c^\dagger_{k\sigma m} c_{k\sigma m} + J\,\mathbf{S}\cdot(\mathbf{J}_{\mathrm{sp},1} + \mathbf{J}_{\mathrm{sp},2})$$

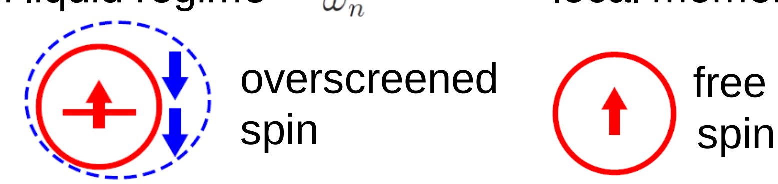


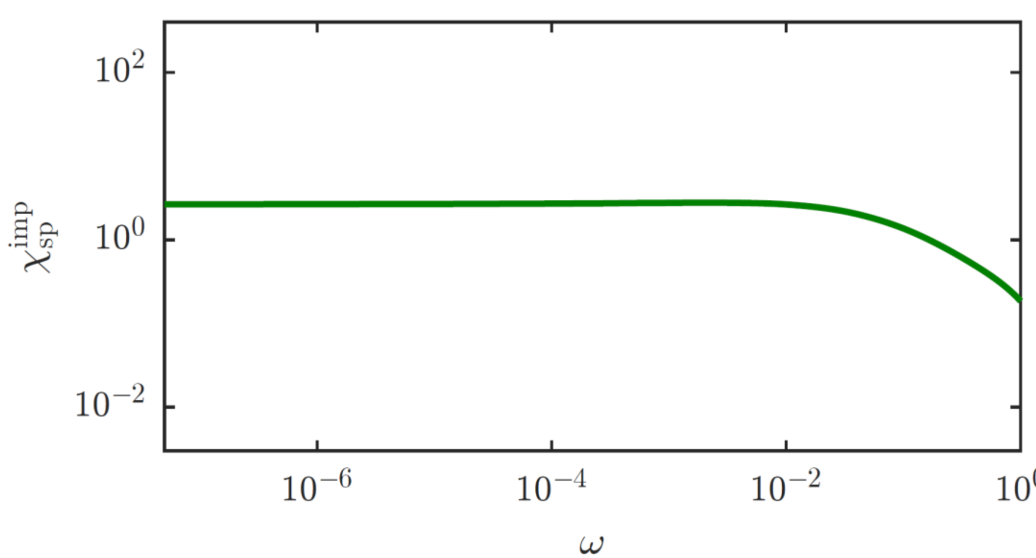








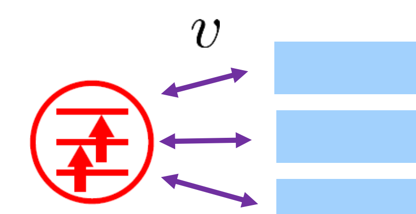




NFL (orbital): 3-channel Anderson-Hund model

$$H_{3\mathrm{AH}} = \sum_{k\sigma}\sum_{m=1,2,3} \varepsilon_k c^\dagger_{k\sigma m} c_{k\sigma m} + v\sum_{k\sigma m}(d^\dagger_{\sigma m} c_{k\sigma m} + c^\dagger_{k\sigma m} d_{\sigma m})$$
$$+ \tfrac{3}{4} J_H \hat{N} + \tfrac{1}{2}(U - \tfrac{1}{2}J_H)\hat{N}(\hat{N}-1) - J_H \mathbf{S}^2$$

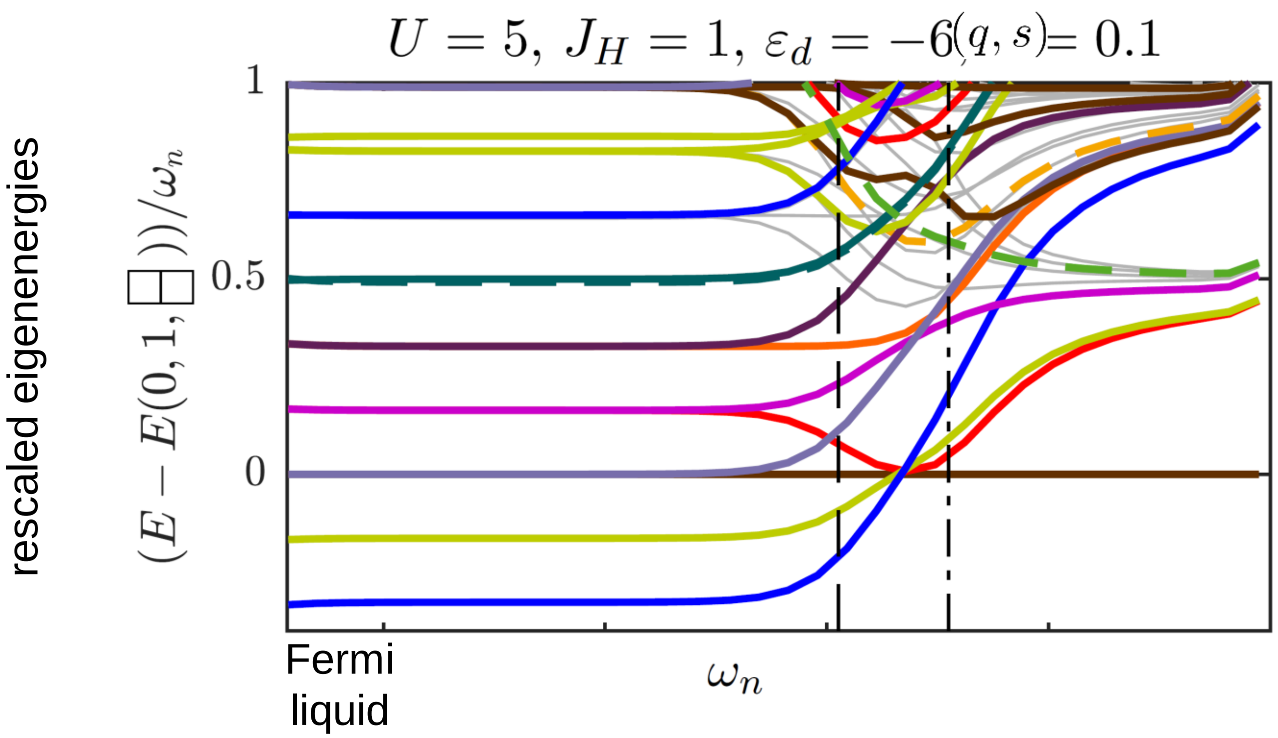
$n_d = 2$

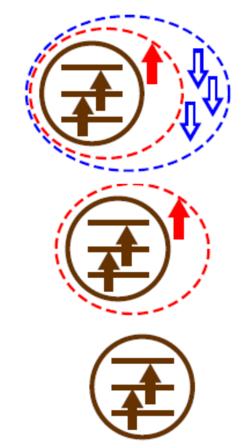


symmetry: $U(1)_{\mathrm{ch}} \times SU(2)_{\mathrm{sp}} \times SU(3)_{\mathrm{orb}}$

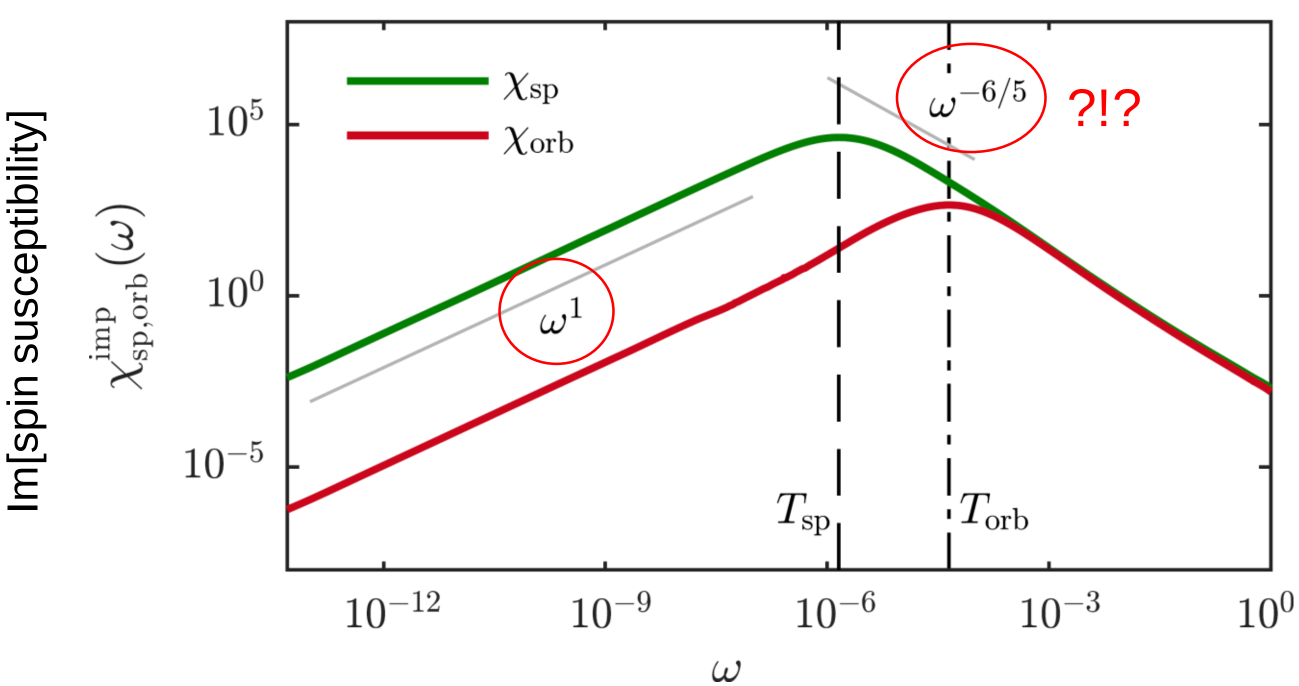
quantum numbers: (q, S, λ)

impurity: $(S, \lambda)_{\mathrm{imp}} = (1, \square)$





$(-2, 0, \bullet)$ (blue)	fully screened
$(+1, \frac{3}{2}, \bullet)$ (red)	orbital singlet
$(0, 1, \square)$ (brown)	free impurity



Spin and orbital susceptibilities:

$\chi_{\mathrm{sp}}(\omega) = \mathrm{Im}\langle \mathbf{S} || \mathbf{S} \rangle_\omega \qquad S^\alpha = d^\dagger_{\sigma m} \sigma^\alpha_{\sigma\sigma'} d_{\sigma' m}$

Pauli matrices

$\chi_{\mathrm{orb}}(\omega) = \mathrm{Im}\langle \mathbf{T} || \mathbf{T} \rangle_\omega \qquad T^a = d^\dagger_{\sigma m} \tau^a_{mm'} d_{\sigma m'}$

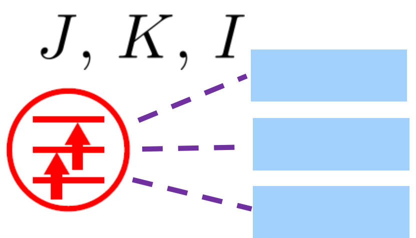
Gell-Mann matrices

ω^1 behavior at low energies: Fermi liquid

spin-orbital separation: $T_{\mathrm{sp}} < T_{\mathrm{orb}}$

NFL (orbital): 3-channel Kondo-Hund model

$$H_{3\mathrm{KH}} = \sum_{k\sigma} \sum_{m=1,2,3} \varepsilon_k c^\dagger_{k\sigma m} c_{k\sigma m} + J_0\, \mathbf{S} \cdot \mathbf{J}_{\mathrm{sp}} + K_0\, \mathbf{T} \cdot \mathbf{J}_{\mathrm{orb}} + I_0\, \mathbf{S} \cdot \mathbf{J}_{\text{sp-orb}} \cdot \mathbf{T}.$$



$$J^\alpha_{\mathrm{sp}} = \sum_{kk'} c^\dagger_{k\sigma m} \sigma^\alpha_{\sigma\sigma'} c_{k'\sigma' m}$$

spin current

$$J^a_{\mathrm{orb}} = \sum_{kk'} c^\dagger_{k\sigma m} \tau^a_{mm'} c_{k'\sigma m'}$$

orbital current

$$J^a_{\text{sp-orb}} = \sum_{kk'} c^\dagger_{k\sigma m} \sigma^\alpha_{\sigma\sigma'} \tau^a_{mm'} c_{k'\sigma' m'}$$

mixed current

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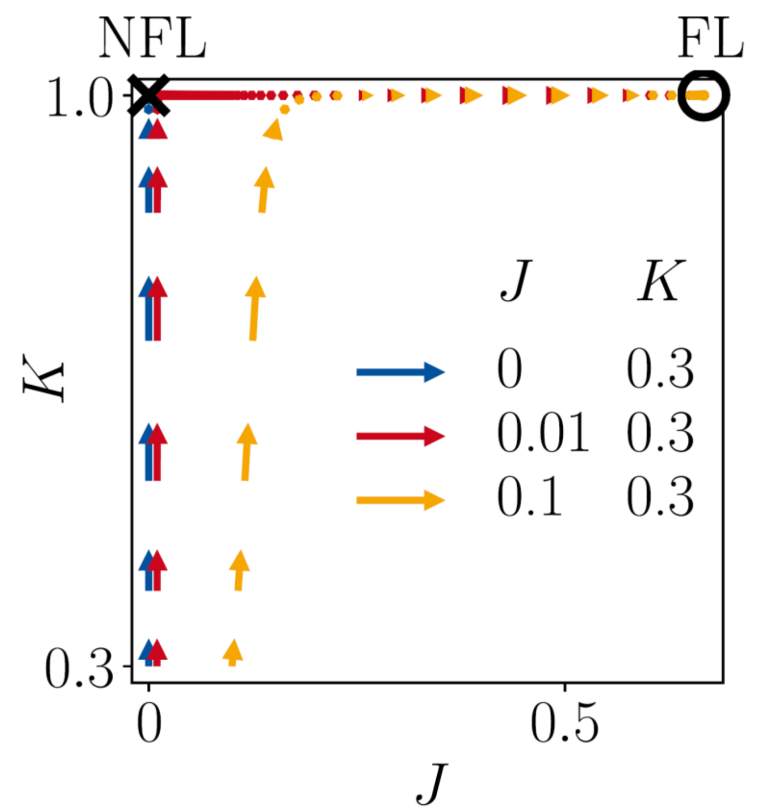
weak-coupling RG flow for $I_0 = 0$

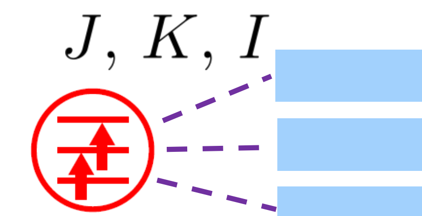


NFL fixed point can be reach by choosing

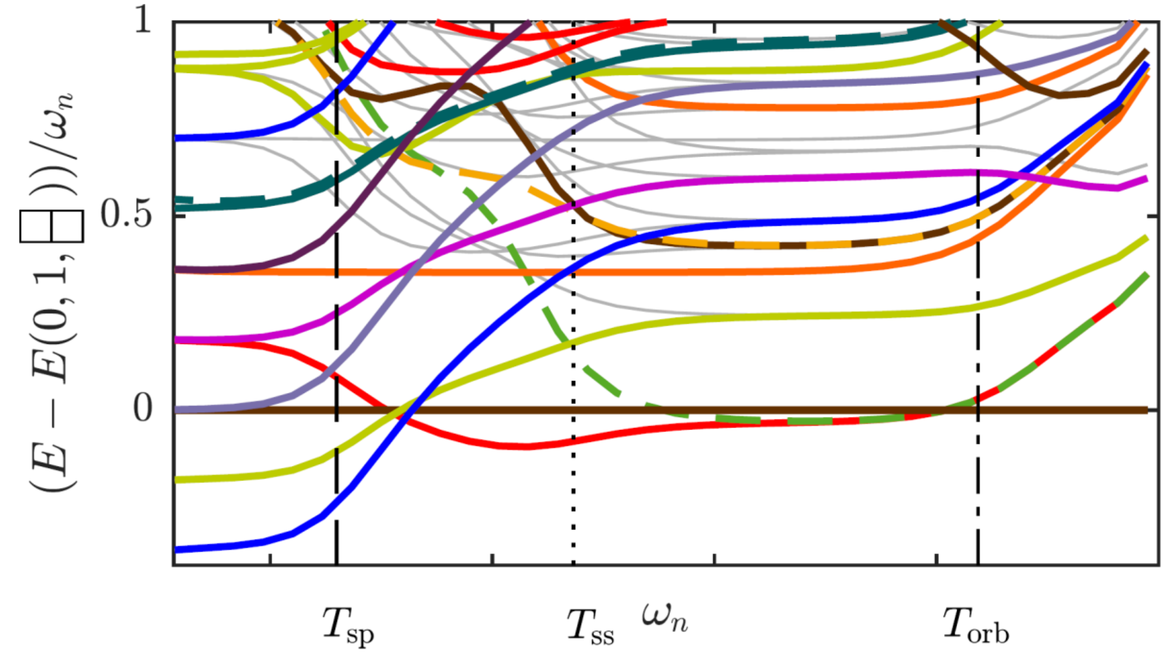
$I_0 = 0,\ J_0 \ll K_0$ then $T_{\mathrm{sp}} \lll T_{\mathrm{orb}}$

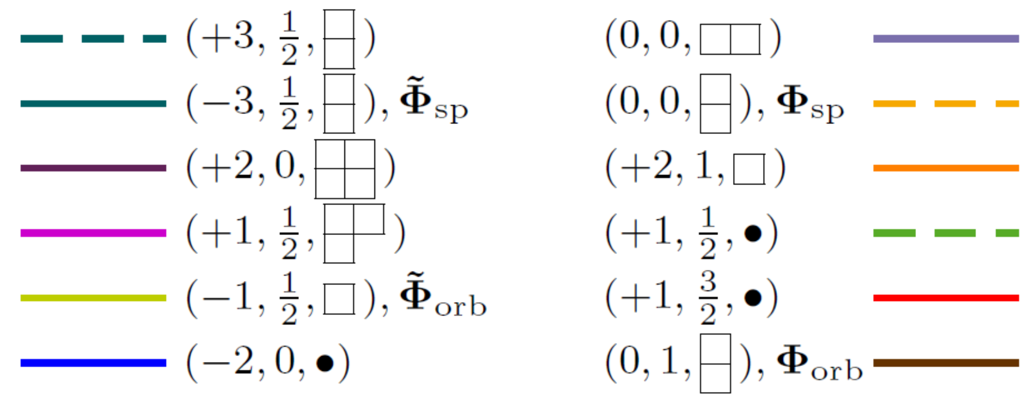
NFL (orbital): 3-channel Kondo-Hund model

$$H_{3\mathrm{KH}} = \sum_{k\sigma} \sum_{m=1,2,3} \varepsilon_k c^\dagger_{k\sigma m} c_{k\sigma m} + J_0\, \mathbf{S}\cdot\mathbf{J}_{\mathrm{sp}} + K_0\, \mathbf{T}\cdot\mathbf{J}_{\mathrm{orb}} + I_0\, \mathbf{S}\cdot\mathbf{J}_{\text{sp-orb}}\cdot\mathbf{T}.$$



$I_0 = 0,\ J_0 = 10^{-4},\ K_0 = 0.3$





Scaling dimensions (from CFT analysis):

$$\Delta_{\mathrm{sp}} = \frac{2}{5},\ \Delta_{\mathrm{orb}} = \frac{3}{5}, \qquad \widetilde{\Delta}_{\mathrm{spin}} = \widetilde{\Delta}_{\mathrm{orb}} = \frac{9}{10}$$

For $\omega > T_{\mathrm{ss}}$, effect of J_0 is very small, and we have:

$$\mathbf{J}_{\mathrm{orb}} \mapsto \Phi_{\mathrm{orb}}, \quad \mathbf{T} \mapsto \Phi_{\mathrm{orb}}, \qquad \mathbf{J}_{\mathrm{sp}} \mapsto \Phi_{\mathrm{sp}}\ , \qquad \mathbf{S} \mapsto \mathbf{S}$$

$$\chi^{\mathrm{imp}}_{\mathrm{orb}} \sim \langle \mathbf{T}\cdot\mathbf{T}\rangle_\omega \mapsto \langle \mathbf{\Phi}_{\mathrm{orb}}\cdot\mathbf{\Phi}_{\mathrm{orb}}\rangle_\omega \sim \omega^{2\Delta_{\mathrm{orb}}-1} \simeq \omega^{1/5}$$

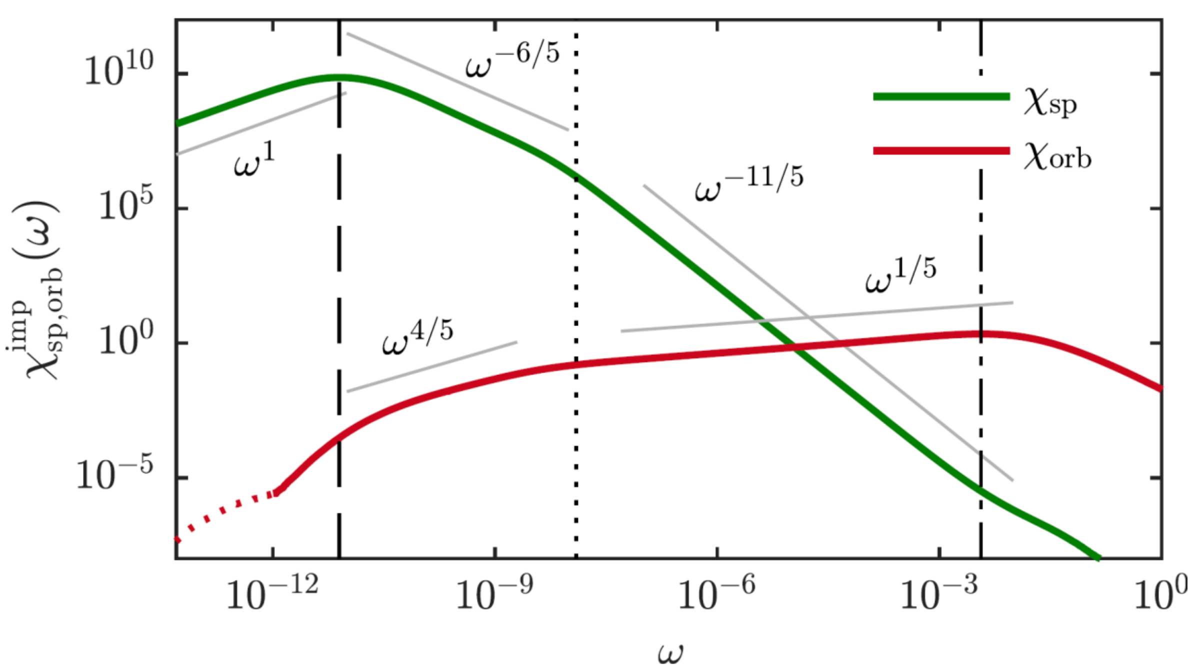
$$\chi^{\mathrm{imp}}_{\mathrm{sp}} \mapsto \langle \mathbf{S}\cdot\mathbf{S}\big(\textstyle\int \mathrm{d}t\, \mathbf{S}\cdot\mathbf{\Phi}_{\mathrm{sp}}\big)^2\rangle_\omega \sim \omega^{2\Delta_{\mathrm{sp}}-3} \simeq \omega^{-11/5}$$

For $\omega < T_{\mathrm{ss}}$, J_0 reshuffles levels and assignments:

$$\mathbf{J}_{\mathrm{orb}} \mapsto \widetilde{\Phi}_{\mathrm{orb}}, \quad \mathbf{T} \mapsto \widetilde{\Phi}_{\mathrm{orb}}, \qquad \mathbf{J}_{\mathrm{sp}} \mapsto \widetilde{\Phi}_{\mathrm{sp}}\ , \qquad \mathbf{S} \mapsto \mathbf{S}$$

$$\chi^{\mathrm{imp}}_{\mathrm{orb}} \sim \langle \mathbf{T}\cdot\mathbf{T}\rangle_\omega \mapsto \langle \widetilde{\mathbf{\Phi}}_{\mathrm{orb}}\cdot\widetilde{\mathbf{\Phi}}_{\mathrm{orb}}\rangle_\omega \sim \omega^{2\widetilde{\Delta}_{\mathrm{orb}}-1} \simeq \omega^{4/5}$$

$$\chi^{\mathrm{imp}}_{\mathrm{sp}} \mapsto \langle \mathbf{S}\cdot\mathbf{S}\big(\textstyle\int \mathrm{d}t\, \mathbf{S}\cdot\widetilde{\mathbf{\Phi}}_{\mathrm{sp}}\big)^2\rangle_\omega \sim \omega^{2\widetilde{\Delta}_{\mathrm{sp}}-3} \simeq \omega^{-6/5}$$



NFL power laws can be explained using CFT [in spirit of Affleck & Ludwig, 1990-1992, using U(1) x $SU(2)_3$ x $SU(3)_2$ Sugawara construction]

Summary

- Minimal 3-band models for Hund metals show spin-orbital separation,
- involving orbital overscreening, leading to non-Fermi-liquid behavior.
- In Anderson-Hund model, the actual NFL fixed point (J=K=0) is not reachable;
- but its properties can be studied using the Kondo-Hund model, where J, K, I can be tuned independently.
- Beatiful NFL power laws were found by NRG and explained by CFT.

Outlook

NRG+DMFT is a highly competitive, powerful, real-frequency, low-energy method !!

- Models without orbital degeneracy: orbital selective Mott transition (feasible, in progress)
- Models with off-diagonal hybridization matrix: spin-orbit scattering (feasible, in progress)
- Real materials (feasible, for three-band models)
- Main limitation: currently feasible for at most three spin-full bands